Entropic Lattice Boltzmann Models
and Quantum Computation
(Final Report for AFOSR Grant FA9550-04-1-0176)

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Abstract

This document is the final report for AFOSR Grant FA9550-04-1-0176, "Entropic Lattice Boltzmann Models and Quantum Computation." Under the terms of this grant, the Center for Quantum Algorithm Design in the Department of Mathematics at Tufts University conducted research on lattice Boltzmann models of hydrodynamics and on quantum lattice algorithms, with emphasis on understanding their interrelationship. We also investigated quantum random walks and the simplification of classical lattice models for hydrodynamics, with the intent of enabling their implementation on quantum computers. Finally, we investigated the applicability of these methods to the problem of turbulence using the dynamical zeta function formalism.

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14. ABSTRACT

This document is the final report for AFOSR Grant FA9550-04-1-0176, "Entropic Lattice Boltzmann Models and Quantum Computation." Under the terms of this grant, the Center for Quantum Algorithm Design in the Department of Mathematics at Tufts University conducted research on lattice Boltzmann models of hydrodynamics and on quantum lattice algorithms, with emphasis on understanding their interrelationship. We also investigated quantum random walks and the simplification of classical lattice models for hydrodynamics, with the intent of enabling their implementation on quantum computers. Finally, we investigated the applicability of these methods to the problem of turbulence using the dynamical zeta function formalism.

15. SUBJECT TERMS

quantum lattice gases, quantum computation, lattice Boltzmann models, entropic lattice Boltzmann models, cellular automata, quantum cellular automata, action principles, periodic orbits, turbulence

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Contents

1   Introduction

This is the final report for AFOSR Grant FA9550-04-1-0176, "Entropic Lattice Boltzmann Models and Quantum Computation." The work was conducted at Tufts University's Department of Mathematics between 2004 and 2008. Section 2 lists the five areas of research enabled by this grant, and describes the principal results and publications in each of these areas. Section 3 lists the personnel supported by this grant, broken down by year. Section 4 describes the publications enabled by and referencing this grant; these include several published works in refereed journals, two PhD theses, and a masters thesis. Section 5 describes the various interactions enabled by this grant. Finally, Sections 6 and Section 7 list new inventions, and awards/honors related to this grant.

2   Accomplishments / New Findings

2.1   Entropic lattice Boltzmann models

The development of entropic lattice Boltzmann models was one of the principal motivations for this project, indeed enshrined in its title. Lattice Boltzmann models of fluid dynamics were introduced in the late 1980s and early 1990s. Since then, they have matured into an important new methodology for computational fluid dynamics, both in academic and industrial settings.

The early development of lattice Boltzmann models was plagued by numerical instabilities that appeared at sufficiently low viscosity. A number of approaches have been taken to tame these instabilities, the most physically motivated being the so-called "entropic" version of the lattice Boltzmann model. This version endows the discrete-velocity kinetic equation with a Lyapunov function, in the spirit of Boltzmann's celebrated H function. From a physical point of view, the Lyapunov function specifies an arrow of time; from a numerical point of view, it ensures the nonlinear numerical stability of the model.

We had published earlier work on entropic lattice Boltzmann models before this project was initiated [1]. During the project's first year, we discovered an entirely new class of such models. In particular, we showed that the requirement of galilean invariance imposes interesting constraints on the form of the Lyapunov function; the Navier-Stokes equations are faithfully reproduced only when the equilibrium distribution function is of Tsallis form. The work has resulted in practical and robust CFD algorithms that remain the focus of active investigation at AFRL, and by a number of groups throughout the world.

Finally, we built a classical computer code to implement this model on parallel processors, and imbedded it in a larger code suite for studying vortex motion in viscous hydrodynamics [2]. This code suite was the focus of much attention in 2005/2006 for its excellent performance on the NSF's TeraGrid. The code is able to initialize the fluid with a wide variety of vortical structures in order to study their interaction and decay. It is parallelized with MPI, and grid-enabled using MPICH-G2 so that it can be run across geographically distributed computational resources. Indeed, the NSF funded a demonstration of this code at the Supercomputing 2005 meeting in Seattle in November of 2005. Moreover the Naval Surface Warfare Center tapped our expertise with lattice Boltzmann models to create of a tool that will predict contaminant dispersion in urban environments.

2.2   Decoherence in lattice models of the Dirac equation

In a discrete-space, discrete-time classical random walk, a particle moves along a regular spatial lattice, tossing a coin to determine where next to move. In a quantum version of such a random walk, the scattering rule (or coin) is given by a general quantum operation, rather than a deterministic unitary or stochastic permutation operation. In the course of our research funded by this grant, we developed a new model for such a quantum random walk that has a unitary noise model. The model includes deterministic unitary and stochastic permutation models, reproducing the Dirac equation and the heat equation respectively, as special cases. It also exhibits interesting intermediate behavior. We demonstrated simulation results confirming this range of behavior by studying the non-unitary diffusive decay of an initial Gaussian pure state. This research resulted in one published paper [3].

Our noise model utilizes a fixed unitary operator coupling a four-dimensional bath to the two-dimensional Hilbert space of the internal degree of freedom of a single quantum lattice gas particle in one spatial dimen-

sion. This distinguishes our work from earlier noise models, such as that given in Kendon et al. [4] in which a single environment qubit is coupled by an interaction with a strength tunable from the case of no coupling to the case where the environment produced a projective measurement of the coin degree of freedom of the quantum random walk.

In our work on this problem, we showed that a two-dimensional environment with a fixed interaction is insufficient to reproduce all possible quantum operations between the bath and the particle. We were able to derive the constraints of parity invariance on the coupling operator for U(N), however, so our work could straightforwardly be extended to include an arbitrarily large environment. For the most general noise model possible, we demonstrated a sampling procedure, wherein randomly sampled unitary operators couple a four-dimensional bath to the internal degree of freedom of the particle, that provably includes all quantum operations.

2.3 Quantum algorithms for mathematical physics

In the first year of this work, we investigated quantum lattice models for the heat equation in which the spatial lattice is represented in the Hilbert space of the quantum system, thereby realizing an idea of Meyer [5]. This approach requires only $\log(N)$ qubits to represent a walk on a lattice of N sites. With 100 qubits, the method could simulate a random walk on a lattice of size 2^{100} far beyond the capabilities of any classical computer.

To implement Meyers suggestion in one spatial dimension, we used a register of $\log(N)$ qubits to represent the position coordinate of a particle on a lattice of size N. To the extent that the register is in a superposition of states, the particle is at a superposition of locations. To make the particle move to the right or left, it was only necessary to add or subtract one from the register, respectively. To include more spatial dimensions, it was only necessary to employ additional registers for the y or z directions.

Tufts Department of Mathematics masters degree student, Nicholas Anzalone, did his masters thesis project on working out an optimal sequence of quantum operations for the study of this model in some detail [6]. In addition, Tufts undergraduate student, Troy Borneman, actually implemented this sequence of operations on an NMR quantum computer in the laboratory of Professor David Cory in the Department of Nuclear Engineering at MIT.

Later in this project, we tried to extend our work in this area to simple hydrodynamic equations of mathematical physics, with mixed success. Quantum lattice-gas models have been proposed in which there is a quantum scattering operation at each site of a spatial lattice. As described, this leads to a range of behaviors wherein the quantum particle is obeying the Dirac equation or the heat equation in physical space. If a lattice of N sites is desired, N qubits and N scattering operations will be necessary.

As noted in the proposal for this grant, a key question that we are addressing is whether or not quantum simulations of various equations of mathematical physics may be fundamentally faster than corresponding classical computations. For example, the simulation of a unit volume of fluid for a unit time requires a computational complexity that scales as the cube of the Reynolds number. This unfavorable scaling makes Direct Numerical Simulation (DNS) of the Navier-Stokes equations currently infeasible for an airplane wing. We wondered if it might be possible to improve this scaling with an appropriate quantum algorithm; this question was another key impetus to the current project.

In the proposal for this grant, we discussed the possibility of accelerating the evolution of reversible CA by diagonalizing its unitary time-development operator. For example, the dynamics of a reversible CA with a total of n bits may be described as a permutation in the state space of $N = 2^n$ dimensions. This may be described by the action of a unitary matrix on a system of n qubits. If it were possible to diagonalize that matrix in a time polynomial in n, we could advance the system arbitrarily many time steps T into the future with a fixed amount of work.

This could never be accomplished on a classical computer, because the time required to diagonalize the time-development matrix, or even to reconstruct the time-development operator for T time steps from the diagonalized matrix, would require more classical operations than the recurrence time of the system. On a quantum computer, however, there is no fundamental reason why this could not be done.

In the third year of research, we constructed unitary time-development operators for variously sized lattices, and sought patterns that would enable us to generalize them to families of quantum circuits. We used various "quantum compilers" for this purpose, as well as the Kaneja-Glaser algorithm. To date, we

have not been able to accomplish this goal, but we continue to work on it beyond the term of this grant. In what follows, we describe some of the progress that we have made.

As promised in the proposal for this grant, for the purposes of this study, we focused on a one-dimensional lattice-gas model of a compressible fluid. The model contains three bits per site, with values $n_j(x, t)$, where $j \in \{-, 0, +\}$. The values of these bits correspond to the presence or absence at position $x \in \mathbb{Z}$ and time t of a particle with velocity -1, 0, or $+1$, and mass 1, 2, or 1, respectively.

At each integer increment of time, the evolution proceeds in two stages: First, the value of the bits collide independently at each site. Since these collisions must conserve mass and momentum, there are only two possibilities for them: If there is no 0 particle at a site, a $\pm$ pair may "bind" together to form a single mass-two particle with velocity 0. Likewise, if there are no $\pm$ particles at a site, a 0 particle may dissociate into two mass-one particles with velocities ± 1. In all other circumstances, the bit values at the site are not altered. Alternatively stated, a collision occurs when the value of the bit

$$C := n_-(1 - n_0)n_+ + (1 - n_)n_0(1 - n_+),$$

is one, in which case all bits are negated. The result of this "collision" step is then

$$
\begin{aligned}
n'_- &= (1 - C)n_- + C(1 - n_-) \\
n'_0 &= (1 - C)n_0 + C(1 - n_0) \\
n'_+ &= (1 - C)n_+ + C(1 - n_+).
\end{aligned}
$$

In the second stage of evolution at a time step, the post-collision values move along the lattice with their associated velocity for one unit of time, retaining their velocity as they do so. The dynamics of this "propagation" step are then described by

$$n_j(x + j, t + 1) = n'_j(x, t).$$

It was first demonstrated by Qian and d'Humières [7] that this model describes a compressible one-dimensional fluid in the appropriate continuum limit.

With N sites and three bits per site, the state space for this model has 2^{3N} states. Because the model conserves mass and momentum, the number of accessible states for generic initial conditions is somewhat lower than this, but it is still exponential in N. Because the dynamics is fully deterministic, they may be described as a permutation on the set of accessible states.

Permutation matrices are straightforward to diagonalize, so we can – in principle, anyway – compute the $2^{3N} \times 2^{3N}$ matrix that accomplishes this. We can also compute the associated diagonal matrix – eigenvalues of permutation matrices are always roots of unity. Finding a quantum circuit for these matrices is very difficult, however, and that problem remains open. We shall continue to work on it in the remaining period of this grant.

There are reasons for optimism in the search for quantum circuits described above. First, if the collision operator is not present, we have shown that the problem is solvable. This result in itself is not trivial. While it may seem that the propagation operation is nothing more than a cyclic shift of certain bits on the lattice, and therefore ought to be accomplishable in order N time, its action in the state space is far more complicated, because the order of the permutation will depend on the starting state. For example, the state 0101 will have period two, while 0001 will have period four. Nevertheless, we have devised a quantum circuit that does this.

The collision operator is also trivially diagonalizable when considered in isolation, because it acts locally on sites. The problem is then that the propagation and collision operators do not commute. (A propagation step followed by a collision will certainly not result in the same state as a collision step followed by a propagation.) This means that the matrix that diagonalizes their product will be substantially different from the matrices that diagonalize them individually.

At this point, we tried to make use of the fact that the ability of the above-mentioned model to describe a one-dimensional compressible fluid is very robust with respect to the exact form of the collision operator. The only really essential features of the collision are that it conserve mass and momentum exactly. It does not even matter if the operator leaves one in a superposition state, as long as all of the superposed states have identical total mass and momentum, and the collision remains spatially local in nature. This flexibility allows us to evade impossibility proofs for problems of this nature, such as the recently proven one for a quantum sieve algorithm for graph isomorphism [8].

We are likely to publish something on this work in the near future. It may or may not be a full solution to the problem, but it will expand on the above insights in substantially greater detail.

2.4 Development of new discrete models of classical mechanics, and quantum analogs thereof

Beginning in the second year of the proposal, a PhD student named Gianluca Caterina was studying quantum lattice models, and wished that he could have a discrete version of Hamilton's Principle of Least Action, so that he could conduct the analog of path-integral quantization. While investigating this, he noted that very little is known about action principles for discrete systems, and this became the focus of his PhD thesis. In particular, he proved a rigorous "No-Go Theorem" for discrete action principles of second-order discrete systems [9, 10]. This work has direct application to path-integral quantization of various kinds of cellular automata and lattice-gas models of dynamics, and we intend to pursue it further in the future.

It is worth describing these results and the history that led to them in a bit more detail for this final report: While it is well known that classical mechanics can be reformulated using the Principle of Least Action, the applicability of action principles to discrete dynamical systems is much less well understood. Recent results have shown that action principles exist and are useful for mechanical systems with a continuous configuration space, but which evolve in discrete time steps; indeed, they are useful in the construction of symplectic integrators for such systems. Much less studied is the situation wherein the configuration space itself is discrete.

Part of the problem is that, for systems with a discrete configuration space, it is impossible to take derivatives with respect to the state variable, so Lagrange's equations no longer make sense. Caterina noted that the Principle of Least Action still makes perfect sense in this situation, however, and he set out to find discrete second-order systems with interesting action principles. Alternatively stated, he was trying to see which – if any – results of classical mechanics would survive if the configuration space were endowed with nothing more than the discrete topology.

At first, thinking that there would be many such examples, we set out to find some using a symbolic mathematics package (Mathematica). We enumerated all second-order dynamical systems with two, three, and four bits per site, and searched them exhaustively for examples with action principles. This in itself was a nontrivial computational task. Of the tens or hundreds of thousands of systems that we studied, we noticed that the subset of such systems that were reversible was disjoint from the subset that admitted an action principle. This result seemed particularly vexing because one's intuition from classical mechanics is just the opposite – it is the reversible systems, described by Lagrange's equations, that are usually reformulated using an action principle.

These computational results seemed too systematic to be a coincidence, so we set about trying to prove them. After much work, we produced a succinct proof of the conjecture. The proof involves the theory of discrete groups and bits of representation theory. The preprint provides numerous examples, so anybody with basic familiarity in discrete group theory can read it.

Finally, we relaxed each of the hypotheses of the proof, and showed that action principles could exist if any of them were not satisfied. In this way, we realized our original goal of finding interesting least-action principles for various discrete dynamical systems. We are now working on using these for discrete path-integral quantization of certain cellular automata.

In the past year, we have nearly completed a new preprint addressing the existence of equivalence classes of cellular automata rules that share the same set of conserved quantities. In particular, we have shown that there exists a binary combiner that takes two cellular automata rules, A and B, and returns a third C, such that C has the same set of conserved quantities as A and B. We have recognized that this theorem is a discrete analog of Noether's Theorem relating symmetries and conserved quantities, and we explain this connection in the paper. We expect this to be submitted for publication soon, and it will acknowledge this grant.

Finally, an exciting possibility raised by Caterina's research is that of the construction of hydrodynamic lattice-gas automata with very small alphabets indeed, perhaps as small as one bit (two states) per site in two dimensions – perfect for simulation on a quantum computer. Toward this end, we have made progress on the problem of identifying which of Hattori and Takesue's conserved quantities [11] may be associated

with mass, momentum, etc. Some of this work was described in Caterina's PhD thesis, and we expect to submit that for journal publication in the coming year. Again, it will acknowledge this grant.

2.5 Lattice Boltzmann algorithm for periodic unstable orbits

Driven dissipative dynamical systems are capable of extremely complicated behavior, even in low dimensions. For example, the Lorenz equations are a system of three ordinary differential equations whose orbits can exhibit chaotic behavior in certain parameter ranges. After an initial transient, the state of the system is drawn to a very complicated subset of all possible states. This subset includes unstable orbits that are periodic (repeat after a time), and it is thought that after a long time the motion remains within the subset, flitting from the vicinity of one unstable periodic orbit to another. That is, each unstable periodic orbit has an associated "stable manifold" that attracts orbits from both inside and outside the attractor, and an "unstable manifold" that repels them while keeping them inside the attractor. Dynamical systems with this behavior are called "hyperbolic."

The importance of unstable periodic orbits in describing the behavior of driven dissipative systems – such as turbulence in a stirred fluid – has been understood since the 1980s [12], and was described in our interim report last year. This result is very nontrivial and unexpected, since the statistics of observables on those orbits themselves are not expected to match their statistics on a "generic" orbit of the dynamical system (over the so-called "natural measure" of the attractor). In spite of this, knowledge of averages over these orbits, as well as other certain characteristics of these orbits (such as their period and monodromy matrix), allow one to discern averages over generic orbits. This is accomplished with the so-called dynamical zeta function formalism [13].

It has also been known since the 1980's that the driven Navier-Stokes equations of fluid dynamics have a finite-dimensional attractor that is replete with unstable periodic orbits (UPOs) of this sort. We believe that these UPOs provide a minimalist description of a turbulent fluid, and we have set out to find them for driven turbulence in two and three dimensions.

During the last two years of this project, my research group and I have developed new ways of locating unstable periodic orbits in dynamical systems of arbitrary dimension. We have tested it on low-dimensional systems, but we are now extending it to dynamical systems with many more degrees of freedom, such as fluids. To do this, quite a bit of numerical analysis was required. In the case of the Navier-Stokes equation, this generalization can be accomplished with the lattice Boltzmann equation. The algorithm begins with an initial guess for a periodic orbit, and simultaneously relaxes both the orbit and the physical time per iteration until it finds a periodic solution. This requires an enormous amount of computer time, and we have applied for and received substantial allocations of time on the NSF's TeraGrid to carry out these studies. At the time of this writing, they are ongoing.

We have produced a preprint on this work that will be sent to a journal very soon. It will acknowledge this grant.

3 Personnel Supported

3.1 2005

1. Prof. Bruce M. Boghosian, Professor of Mathematics and Adjunct Professor of Computer Science, Department of Mathematics, Tufts University.

2. Dr. Peter J. Love, Postdoctoral Associate, Department of Mathematics, Tufts University. (Presently, Senior Applications Scientist, D-Wave Systems, Inc., Vancouver, Canada.)

3. Mr. Lucas Finn, PhD student, Department of Mathematics, Tufts University.

4. Mr. Nicholas Anzalone, Masters student, Department of Mathematics, Tufts University.

5. Mr. Christopher Kottke, former Undergraduate Student, Departments of Mathematics and Physics, Tufts University. (Will begin graduate studies at the MIT Department of Mathematics, fall, 2005.)

6. Mr. Troy Borneman, former Undergraduate Student, Department of Electrical Engineering, Tufts University. (Will begin graduate studies with Prof. David Cory at the MIT Department of Nuclear Engineering, fall, 2005.)

7. Mr. Alejandro Taylor-Escribano, Undergraduate Student, Department of Mathematics, Tufts University.

3.2 2006

1. Prof. Bruce M. Boghosian, Professor and Chair of Mathematics and Adjunct Professor of Computer Science, Department of Mathematics, Tufts University.

2. Prof. Peter J. Love, Haverford College, Pennsylvania.

3. Mr. Lucas Finn, PhD student, Department of Mathematics, Tufts University.

4. Mr. Christopher Kottke, former Undergraduate Student, Departments of Mathematics and Physics, Tufts University. (Will begin graduate studies at the MIT Department of Mathematics, fall, 2005.)

5. Mr. Ian Duffy, Masters Student, Department of Mathematics, Tufts University.

6. Mr. Alejandro Taylor-Escribano, Undergraduate Student, Department of Mathematics, Tufts University.

3.3 2007

1. Prof. Bruce M. Boghosian, Professor and Chair of Mathematics and Adjunct Professor of Computer Science, Department of Mathematics, Tufts University.

2. Dr. Jonas Lätt, Postdoctoral Associate, Department of Mathematics, Tufts University.

3. Mr. Ian Duffy, Masters Student, Department of Mathematics, Tufts University.

4. Ms. Hui Tang, Graduate Student, Department of Mathematics, Tufts University.

5. Mr. Aaron Brown, Graduate Student, Department of Mathematics, Tufts University.

6. Mr. Alejandro Taylor-Escribano, Undergraduate Student, Department of Mathematics, Tufts University.

7. Mr. Luis Fazendeiro, Graduate Student, University College London (travel support for a visit to Tufts University).

4 Publications

4.1 Refereed Publications

4.1.1 2005

The following publications were done during the period covered by this report, and have been published or accepted for publication:

1. Lucas I. Finn, Bruce M. Boghosian, Christopher N. Kottke, "Vortex Core Identification in Viscous Hydrodynamics," *Phil. Trans. Royal Soc. A* **363** (2005) 1937-1948 [14].

2. Lucas I. Finn, Bruce M. Boghosian, "A Variational Approach to Vortex Core Identification," *Physica A* **362** (2006) 11-16 [15].

3. Peter J. Love, Bruce M. Boghosian, "From Dirac to Diffusion: Decoherence in Quantum Lattice Gases," *J. Quantum Information Processing* **4** (2005) 335-354 [16].

4. Bruce M. Boghosian, "General Theory of Galilean-Invariant Entropic Lattice Boltzmann Models," in the *Proceedings of the 31st Workshop of the International School of Solid State Physics on Complexity, Metastability and Nonextensivity* at the Ettore Majorana Foundation and Centre for Scientific Culture in Erice, Sicily (20-26 July 2004) [17].

5. Peter J. Love, Bruce M. Boghosian, "Type II Quantum Algorithms," *Physica A* **362** (2006) 210-214 [18].

6. David J. Fair, Rakesh Venkatesh, Bruce Boghosian, and Douglas M. Matson, "Role of Sample Size in Nucleation Kinetics of Phase Transformations in Steel Alloys," *Microgravity Science and Technology Journal* XVI-1(2005) 55 [19].

4.1.2 2006

The following publications were done during the period covered by this report, and have been published or accepted for publication:

1. B. Boghosian, P. Coveney, S. Dong, L. Finn, S. Jha, G. Karniadakis, N. Karonis, "Nektar, SPICE, and Vortonics: Using Federated Grids for Large-Scale Scientific Applications," in *Proceedings of Challenges of Large Applications in Distributed Environments (CLADE)*, published by the IEEE Computing Society (19 June 2006) 34-42. ISBN 1-4244-0420-7. INSPEC Accession Number 9018016 [20].

2. Bruce M. Boghosian, Jean Pierre Boon, "Lattice Boltzmann and Nonextensive Diffusion," *Europhysics News* **36** (6) (November/December 2005) 192-194 [21].

4.1.3 2007

The following publications were done during the period covered by this report, and have been published or accepted for publication:

1. A. Xu, S. Succi, B.M. Boghosian, "Lattice BBGKY Scheme for Two-Phase Flows: One-Dimensional Case," in Proceedings of 14th International Conference on the Discrete Simulation of Fluid Dynamics (DSFD 2005), published in *Mathematics and Computers in Simulation* **72** (2006) 249-252 [22].

4.2 Unpublished Documents

4.2.1 2005

The following works were completed but not published. The first is a student's masters' thesis, while the second is a *proposal* for a paper to the journal *Physics Reports* (which publishes scientific papers only by prior arrangement).

1. N. Anzalone, "Designing a Quantum Circuit for Modeling the Heat Equation," masters thesis, Department of Mathematics, Tufts University (2005) [6].

4.2.2 2006

The following work was completed but not published. It is a student's PhD thesis.

1. L.I. Finn, "Vortex Core Identification in Viscous Hydrodynamics," PhD Dissertation, Department of Mathematics, Tufts University (2006) [2].

4.2.3 2007

The following three works are as yet unpublished. The first is still in a referee process, and we are reasonably confident of a positive outcome. The second is a student's PhD thesis. The third and fourth are in late stages of preparation:

1. G. Caterina, B.M. Boghosian, "A No-Go Theorem for the Existence of an Action Principle for Discrete Invertible Dynamical Systems," preprint `http://arxiv.org/abs/nlin.CG/0611058` .

2. G. Caterina, "Least Action Principles and Additive Invariants for a Class of Reversible Cellular Automata," PhD dissertation, Department of Mathematics, Tufts University (2007) [10].

3. B.M. Boghosian, A. Brown, J. Lätt, J. Tam, H. Tang, P.V. Coveney, L. Fazendeiro, "New Variational Principles for Locating
Periodic Orbits of Differential Equations," in preparation (2008).

4. G. Caterina, B.M. Boghosian, "An order-preserving property of additive invariant for Takesue-type reversible cellular automata," in preparation (2008).

5 Interactions / Transitions

5.1 Meetings and Conferences

This project was represented at all of the conferences listed below.

5.1.1 2005

1. Speaker and Member of Organizing Committee, 14th International Conference on the Discrete Simulation of Fluid Dynamics (DSFD 2005), Kyoto, Japan (22-26 August 2005).

2. Speaker, "Entropic Lattice Boltzmann Models," Third M.I.T. Conference on Computational Fluid and Solid Mechanics, Massachusetts Institute of Technology (14-17 June 2005).

3. Speaker, "A Variational Principle for Vortex Core Identification," Conference on Vortex Rings and Filaments in Classical and Quantum Systems, International Centre for Theoretical Physics, Trieste, Italy (6-8 June 2005).

4. Speaker, "Entropic Lattice Boltzmann Models," 93rd Statistical Mechanics Conference, Rutgers University, Piscataway, New Jersey (15-17 May 2005).

5. Speaker, Physics Department Colloquium, Clark University, Worcester, Massachusetts (3 March 2005).

6. Speaker, Center for Computational Science, Boston University (4 March 2005).

7. Speaker, Workshop on Quantum Computing for Physical Modeling, Martha's Vineyard, Massachusetts (12-15 September 2004).

8. Speaker and Member of Organizing Committee, 13th International Conference on the Discrete Simulation of Fluid Dynamics (DSFD 2004), Cambridge, Massachusetts, USA (16-20 August 2004).

9. Speaker, International Conference on Computational and Experimental Engineering and Sciences (ICES 2004), Madeira, Portugal (26-29 July 2004).

10. Speaker, 31st Workshop of the International School of Solid State Physics, "Complexity, Metastability and Nonextensivity," Ettore Majorana Foundation and Centre for Scientific Culture, Erice, Sicily (20-26 July 2004).

11. Speaker, RealityGrid Annual Conference, Royal Society of London (15-16 June 2004).

5.1.2 2006

1. Speaker, Dynamics Seminar, Brown University (17 April 2006).

2. Speaker, Center for Computational Science, Boston University (7 April 2006).

3. Speaker, SIAM Conference on Parallel Computing, San Francisco, California (to be held, 22-24 February 2006).

4. Speaker, Department of Applied Mathematics Colloquium, Brown University (29 November 2005).

5. Speaker at booths for TeraGrid, Pittsburgh Supercomputing Center, Argonne National Laboratory, and UK eScience Programme at Supercomputing 2005, Seattle, Washington (12-17 November 2005).

6. Speaker, 14th International Conference on the Discrete Simulation of Fluid Dynamics (DSFD 2005), Kyoto, Japan (22-26 August 2005).

5.1.3 2007

1. Colloquium Speaker, Shanghai Institute of Applied Mathematics and Mechanics, Shanghai University, Shanghai, China (6 December 2007).

2. Speaker, 16th International Conference on the Discrete Simulation of Fluid Dynamics (DSFD 2007), Banff, Alberta, Canada (23-27 July 2007).

3. Colloquium Speaker, Manchester Centre for Interdisciplinary Computational and Dynamical Analysis (CICADA), University of Manchester, Manchester, United Kingdom (27 June 2007).

4. Speaker, "Computational Science 2007: Interdisciplinary Challenges and Perspectives, from the Grid to e-Science," Royal Society of London (25-26 June 2007).

5. Speaker, "Quantum Algorithms for Classical Physics Problems and Differential Equations," workshop held at Los Alamos National Laboratory, Los Alamos, New Mexico (24-27 May 2007).

6. Poster, "Dynamics Days," Boston, Massachusetts (3-6 January 2007).

7. Speaker, "Expanding Horizons: The Scientific Legacy of Brosl Hasslacher," Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico (3-4 November 2006).

5.2 Consultative and Advisory Functions

During the course of this project, Bruce Boghosian was a Visiting Fellow at the Centre for Computational Science at University College London. He was also a Visiting Faculty member in the College of Engineering at Peking University in China, and in the dynamo research group at the École Normale Supérieure in Paris. He was a consultant with MesoSoft Corporation of Lexington, Massachusetts, under contract to Exa Corporation and also to Interactive Supercomputing Corporation.

5.3 Transitions

The following transitions took place during the course of this project:

1. Our lattice Boltzmann code was shown to be very effective for the study of vortex interactions [2]. The National Science Foundation funded a public demonstration of this code at the Supercomputing 2005 meeting in Seattle, Washington during November, 2005. This demonstration was very successful, and the NSF has awarded us substantial allocations of computer time on the TeraGrid ever since.

2. Bruce Boghosian worked on a project initiated by the Naval Surface Warfare Center to employ lattice Boltzmann models of fluids to create a tool to predict contaminant dispersion in urban environments. The PI of this effort was Dr. George Andrews, Lead Scientist of Chemical, Biological, and Radiological Defense at the NSWC. Another co-PI was Dr. Hudong Chen of Exa Corporation. The lattice Boltzmann expertise gained as part of this project was thereby transfered to use for the national defense.

3. Dr. Peter J. Love, a postdoctoral researcher funded by this grant at Tufts University, took the position of Senior Applications Scientist at D-Wave Systems, Inc., a start-up company in Vancouver, Canada devoted to commercial applications of quantum computation. Subsequently, he took a tenure-track assistant professorship in the Department of Physics at Haverford College in Pennsylvania.

4. Dr. Lucas Finn, a graduate student who received his PhD in the Department of Mathematics at Tufts University working on this project, accepted a staff scientist position at BAE Systems in Burlington, Massachusetts.

5. Dr. Gianluca Caterina, a graduate student who received his PhD in the Department of Mathematics at Tufts University working on this project, took a postdoctoral position at Northeastern University, and subsequently a full-time faculty position at Endicott College.

6 Discoveries, Inventions, Patent Disclosures

No inventions or patent disclosures have arisen from this project.

7 Honors / Awards

During 2005, our collaboration with British researchers on high-performance scientific computational fluid dynamics was chosen to be featured on the web page of the British Embassy to the United States. (See

`http://www.britainusa.com/science/information_communication_technology/article.asp?a=7648`

for more details.)

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